WHAT IS CLAIMED IS:

1. A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to tests of interactions between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target; and

a user interface allowing a user to view the selected compound and to selectively view information from the first database, the second database, and the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database.

2. The computer system of claim 1, wherein the interaction includes binding and the effect includes inhibitory effect.

3. The computer system of claim 1, wherein the chemical compounds include compounds with no known biological activity or that have failed in tests.

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4. The computer system of claim 1, wherein the chemical compounds include compounds tested in animals.

5. The computer system of claim 1, wherein the chemical compounds include compounds known to have an effect on the environment.

6. The computer system of claim 1, wherein the chemical compounds include pharmacological reference agents.

7. The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals in the market for clinical use for which there is a substantial amount of biological information available.

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8. The computer system of claim 1, wherein the chemical compounds include compounds approved for testing in humans.

9. The computer system of claim 1, wherein the chemical compounds include compounds obtained from natural resources that exhibit biological activity.

10. The computer system of claim 1, wherein the molecular targets include receptors.

11. The computer system of claim 1, wherein the molecular targets include enzymes.

12. The computer system of claim 1, wherein the molecular targets include nucleic acids.

13. The computer system of claim 1, wherein the molecular targets include carbohydrates.

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14. The computer system of claim 1, wherein the records of the first database corresponding to a plurality of chemical compounds are organized in categories related to the description and properties of the compounds.

15. The computer system of claim 14, wherein the categories include:

compound name;

compound type;

physical-chemical characteristics;

chemical space coordinates or structural descriptors; and

solubility.

16. The computer system of claim 1, wherein the first database includes a natural product database.

17. The computer system of claim 1, wherein the first database includes a failed drug database.

18. The computer system of claim 1, wherein the first database includes a chemical registry database.

19. The computer system of claim 1, wherein the second database includes a three-dimensional structure database.

20. The computer system of claim 1, wherein the second database includes a sequence/mutation database.

21. The computer system of claim 1, wherein the second database includes a genomic database.

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22. The computer system of claim 1, wherein the records in the third database corresponding to biological information related to the chemical compounds effects on the biological targets, are organized in categories that include:

compound name;

target name;

toxicity;

side effects; and

mechanism of drug action.

23. The computer system of claim 1 further comprising means for setting an interaction test threshold corresponding to said effect and means for selecting the compound when its use results in a test meeting the interaction test threshold.

24. A method for analyzing data relevant to drug discovery and development comprising:

selecting chemical compounds from a first database containing records corresponding to a plurality of chemical compounds;

selecting molecular targets from a second database containing records corresponding to a plurality of molecular targets;

producing information corresponding to the interactions between each of the selected chemical compounds and each of the selected molecular targets;

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selecting a biological activity from a third database containing records corresponding to biological information related to effects of chemical compounds on biological targets; and

using the produced information to correlate patterns of interactions between chemical compounds and molecular targets associated with the selected biological activity.

25. The method of claim 24, wherein the step of producing information includes the steps of:

generating binding data of the binding between each of the selected chemical compounds and each of the selected molecular targets by monitoring the inhibitory effect that an unknown compound has on said binding;

setting a binding test threshold corresponding to the inhibitory effect; and

generating information on the combination of unknown compound, molecular target, and chemical compound that meets or fails to meet the binding test threshold.

26. The method of claim 25, wherein the binding data comprises positive and negative binding information.

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